

SPPLEMENTARY MATERIAL

Article

Benzophenones from *Anemarrhena asphodeloides* Bge. Exhibit Anticancer Activity in HepG2 Cells via the NF- κ B Signaling Pathway

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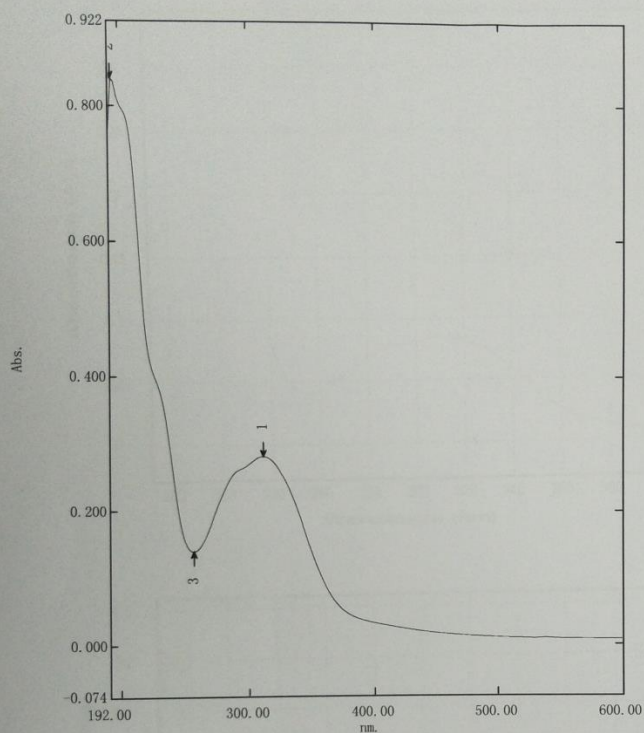
Figure S1.9 Calculating OR spectra of compound **1**

Table S1 Growth inhibition of HepG2 and Hep3B cells in the presence of different compounds after 72 h incubation (IC₅₀ values in nM).

光谱峰值检测报告

2019/02/28 13:41:58

数据集: ZLZD-23 - RawData



[测定属性]
 波长范围 (nm): 192.00 到 600.00
 扫描速度: 中速
 采样间隔: 0.5
 自动采样间隔: 启用
 扫描模式: 单个

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 仪器类型: UV-2700 系列
 测定方式: 吸收值
 狭缝宽: 5.0 nm
 积分时间: 0.1 秒
 光源转换波长: 323.0 nm
 检测器单元: 直接
 S/R 转换: 标准
 阶梯校正: OFF

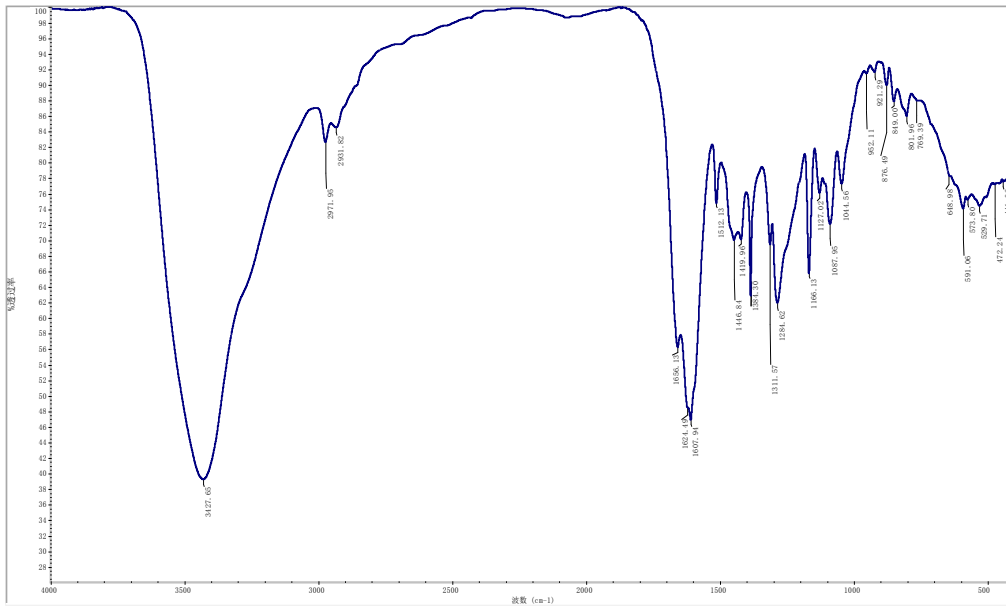
[附件属性]
 附件: 无

[数据处理参数]
 阈值: 0.0010000
 点: 4
 内插: 停用
 平均: 停用

[样品准备属性]
 重量: 0.67mg
 体积: 1ml
 稀释: 30倍
 光程长: 10mm
 附加信息: 2019/02/28 13:38:06
 ZLZD-23 MeOH

No.	P/V	波长 (nm)	Abs.	描述
1	●	311.50	0.284	
2	●	194.50	0.839	
3	●	257.00	0.140	

Figure S1.1 UV spectrum of compound 1



Sample Name: ZLZD-23
 KBr压片
 采集时间: 星期一 3月 04 15:37:04 2019 (GMT+08:00)
 仪器型号: NICOLET iS10
 Software version: OMNIC 9.8.372

样品扫描次数: 16
 背景扫描次数: 16
 分辨率: 4.000
 采样增益: 1.0
 动镜速度: 0.4747
 光阑: 80.00

星期一 3月 04 15:46:25 2019 (GMT+08:00)

标峰:
 谱图: ZLZD-23
 范围: 4000.00 400.00
 (绝对) 阈值: 93.933
 灵敏度: 99

峰位置:	强度:
441.06	77.473
472.24	77.122
529.71	74.364
573.80	75.166
591.06	74.004
801.96	85.951
849.00	87.792
876.49	89.907
921.29	91.546
952.11	91.399
1044.56	77.244
1087.95	72.028
1127.02	75.998
1166.13	65.657
1284.62	61.904
1311.57	69.360
1384.30	62.790
1419.96	70.042
1446.84	69.981
1512.13	74.699
1607.94	46.798
1656.13	56.180
2931.82	84.468
2971.95	82.594
3427.65	39.160

Figure S1.2 IR spectrum of compound 1

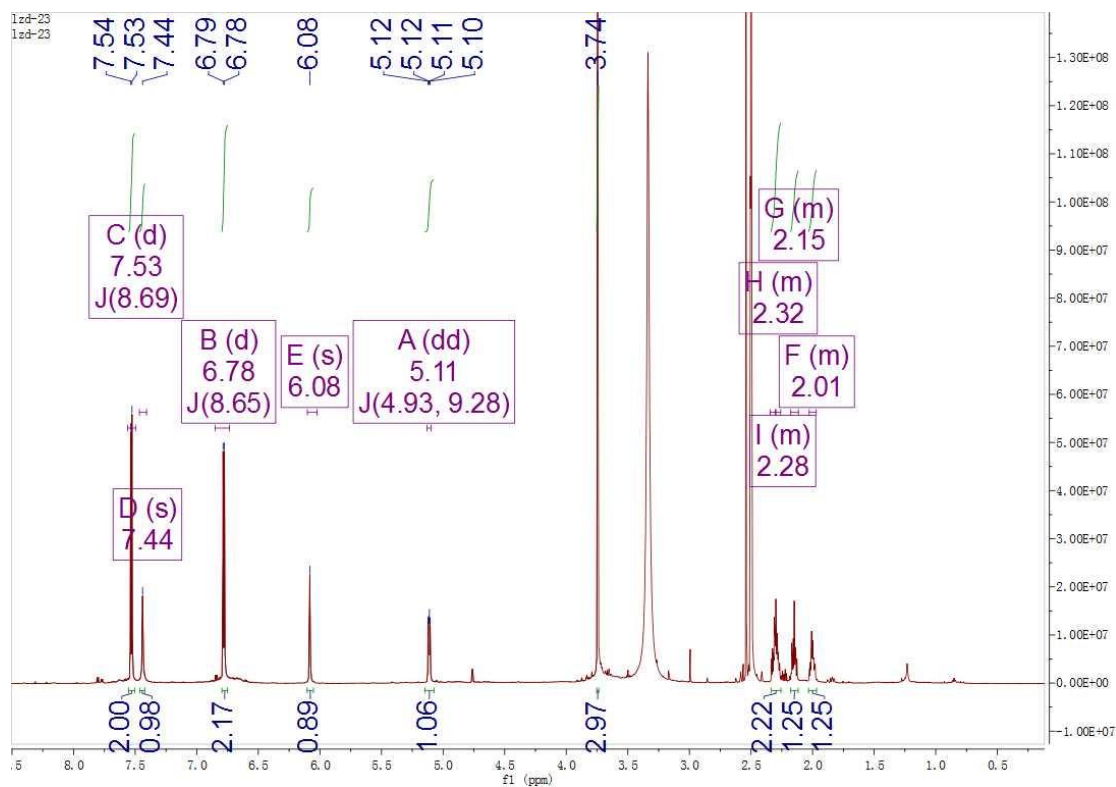


Figure S1.3 ^1H NMR spectrum (800 MHz, $\text{DMSO-}d_6$) of compound **1**

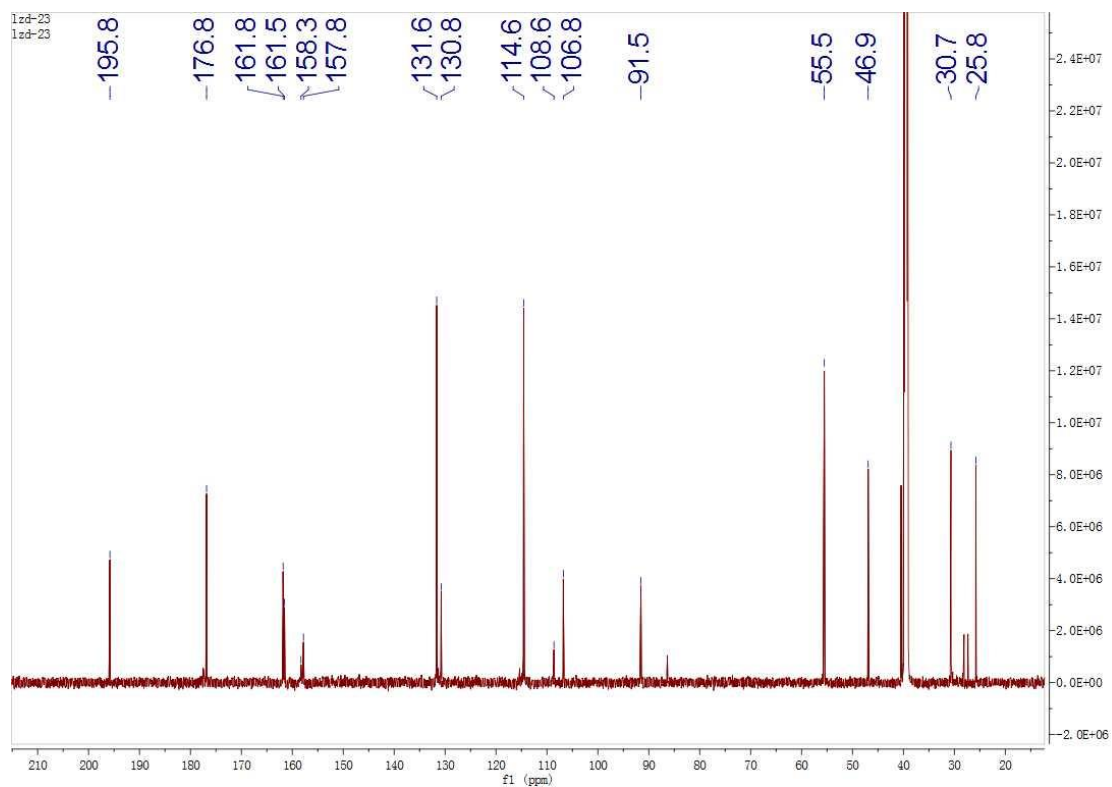


Figure S1.4 ^{13}C NMR spectrum (200 MHz, $\text{DMSO-}d_6$) of compound **1**

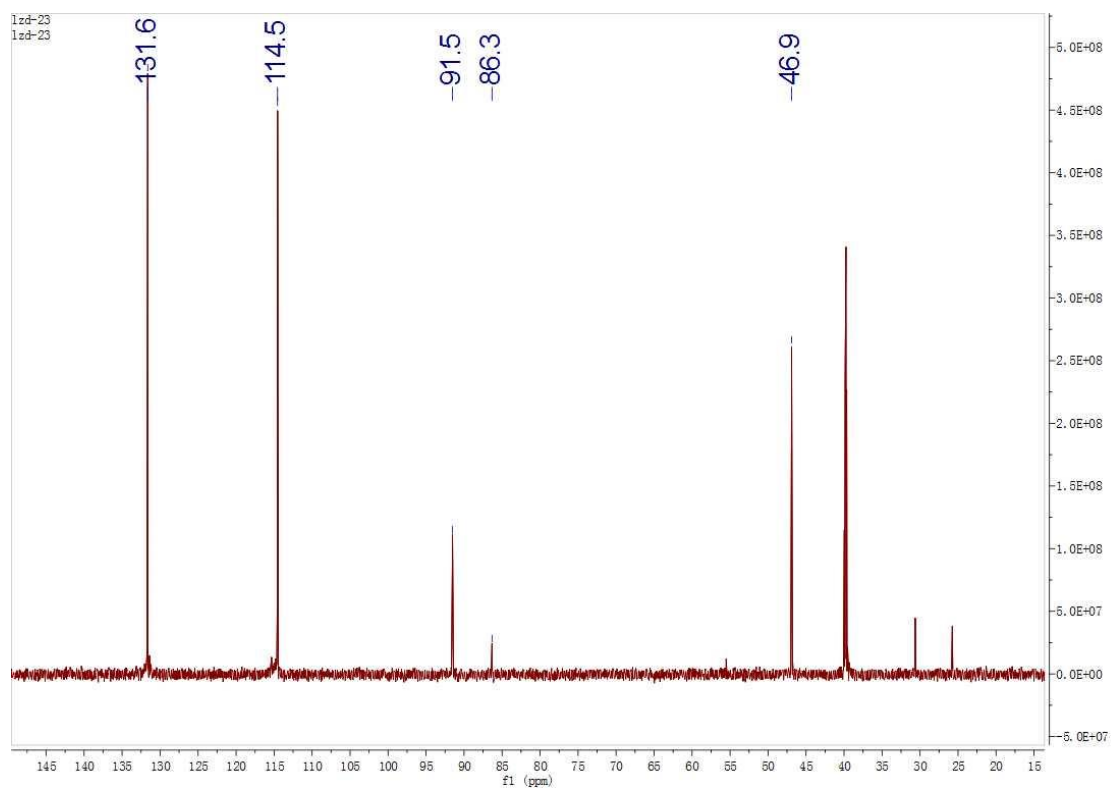
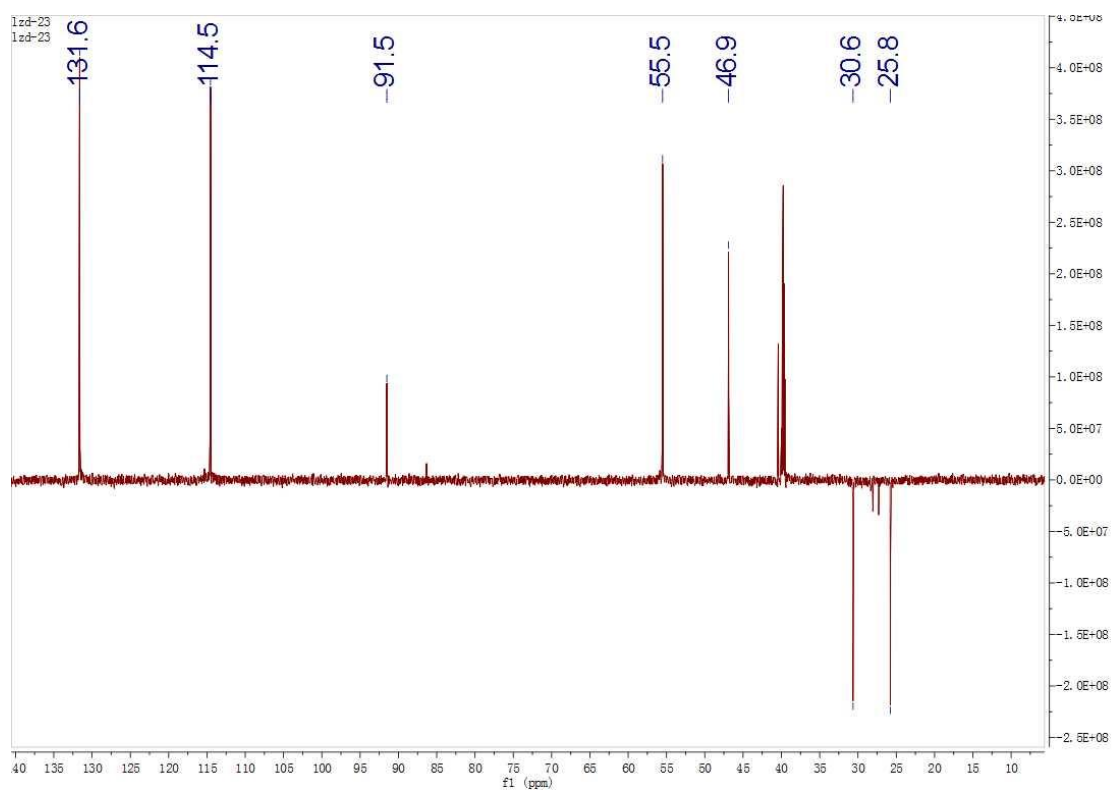


Figure S1.5 DEPT spectrum (200 MHz, DMSO-*d*₆) of compound **1**

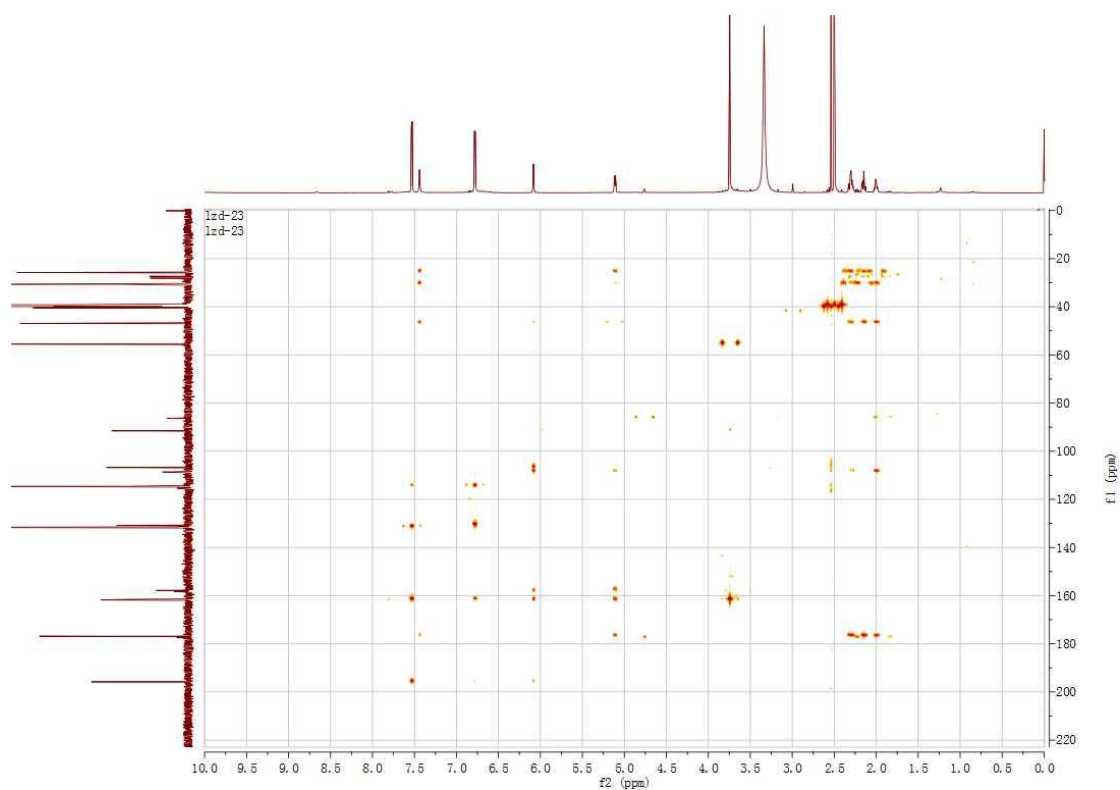


Figure S1.6 HMBC spectrum (800 MHz, DMSO-*d*₆) of compound **1**

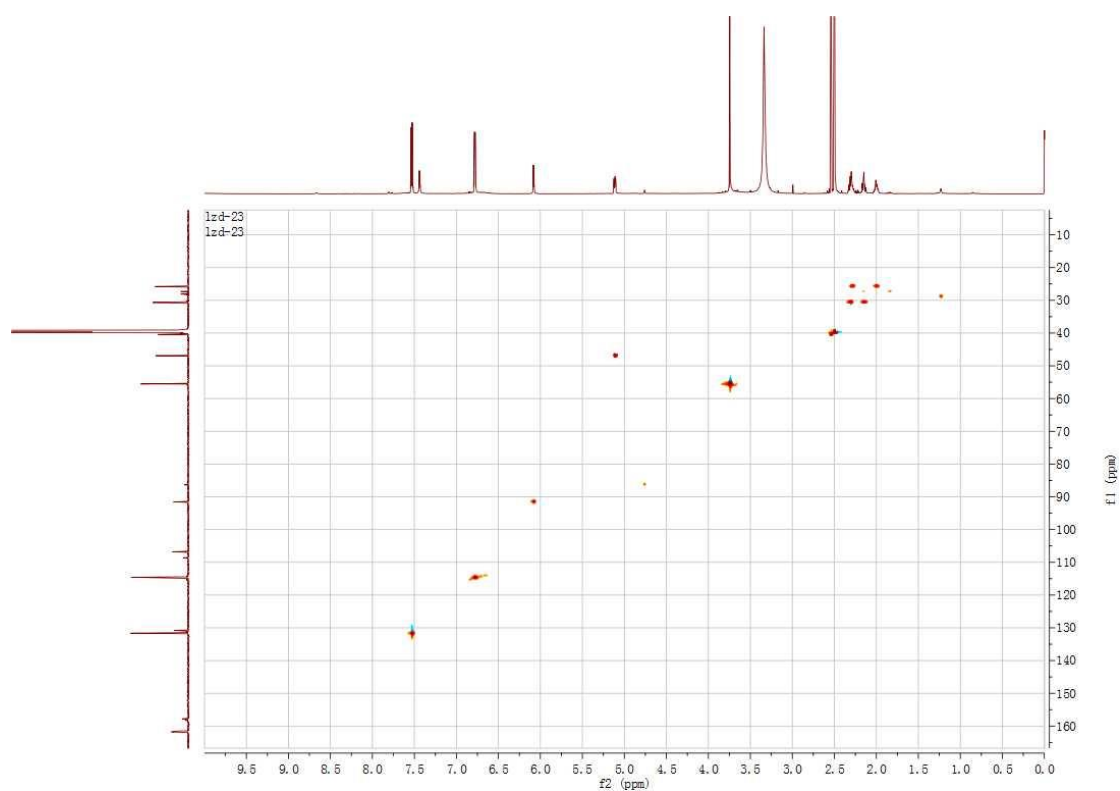


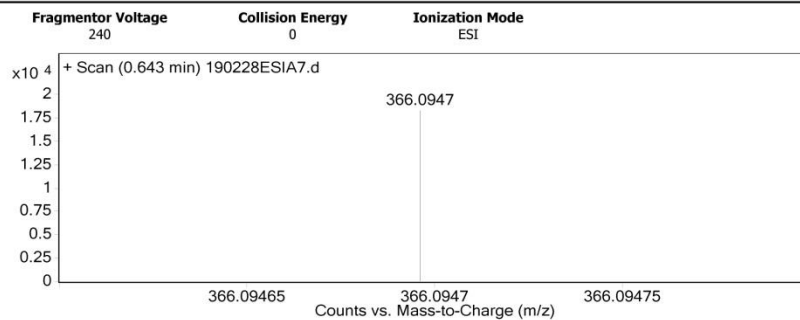
Figure S1.7 HSQC spectrum (800 MHz, DMSO-*d*₆) of compound **1**

Qualitative Analysis Report

Data Filename	190228ESIA7.d	Sample Name	zld-23
Sample Type	Sample	Position	
Instrument Name	Agilent G6230 TOF MS	User Name	KIB
Acq Method	ESI.m	Acquired Time	2/28/2019 10:31:36 AM
IRM Calibration Status	Success	DA Method	ESI.m
Comment			

Sample Group		Info.
Acquisition SW	6200 series TOF/6500 series	
Version	Q-TOF B.05.01 (B5125.2)	

User Spectra



Peak List

<i>m/z</i>	<i>z</i>	Abund	Formula	Ion
121.0509	1	28154.41		
312.362	1	9971.65		
366.0947	1	18319.05	C18 H17 N Na O6	M+
367.1006	1	43828.62		
407.1217	1	11287.66		
408.1277	1	26718.01		
409.161	1	34730.88		
710.2071	1	17512.92		
711.2116	1	27672.05		
922.0098	1	29409.73		

Formula Calculator Element Limits

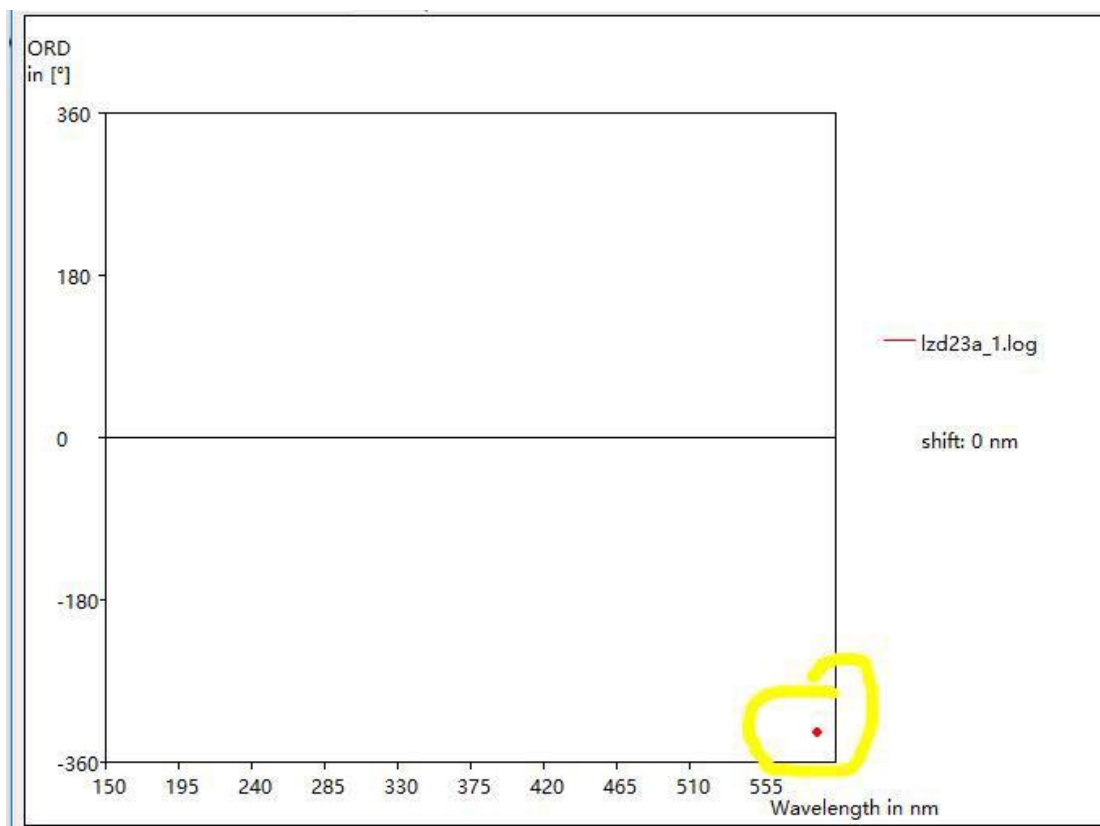
Element	Min	Max
C	0	200
H	0	400
O	0	10
Na	1	1
N	1	1

Formula Calculator Results

Formula	CalculatedMass	Mz	Diff. (mDa)	Diff. (ppm)	DBE
C18 H17 N Na O6	366.0954	366.0947	0.7	1.8	10.5

--- End Of Report ---

Figure S1.8 HRESIMS spectrum of compound **1**



```

dimension 70 with 3 vectors. FullF1: Do perturbations 1 to 3. Dipole-
magnetic dipole polarizability for W= 0.077318:
3 1 0.154262D+02 0.164532D+02 -0.395992D+02 2 0.443034D+02 -0.960516D+02
-0.351420D+02 3 -0.401683D+03 -0.432994D+02 0.893424D+02 w= 0.077318 a.u.,
Optical Rotation Beta= -2.9057 au. Molar Mass = 343.3354 grams/mole, [Alpha] (
5893.0 Å) = -327.12 deg. End of Minotr F.D. properties on file 721 Mask= 2
NFrqRd= 1 NDeriv= 1 ND12= 1 LenFil= 12: Frequencies= 0.077318 Property
number 2 -- FD Optical Rotation Tensor frequency 1 0.077318:
2 3 1 0.154262D+02 0.164532D+02 -0.395992D+02 2 0.443034D+02
-0.960516D+02 -0.351420D+02 3 -0.401683D+03 -0.432994D+02 0.893424D+02 End of Minotr
F.D. properties file 722 does not exist. End of Minotr F.D. properties file 788 does
not exist. Leave Link 1002 at Wed Apr 17 21:11:08 2019, MaxMem= 4294967296 cpu:
34438.2 (Enter /soft/apps/Paid//g09/1601.exe) Copying SCF densities to generalized density
rwf, IOpCl= 0 IROHF=0.
*****

```

$[\alpha]_D^{25}$ -327.12 (*c* 0.10, MeOH) (calculated OR)

Figure S1.9 Calculating OR spectra of compound **1**

Table S1 Growth inhibition of HepG2 and Hep3B cells in the presence of different compounds after 72 h incubation (IC50 values in nM).

compounds	Cells IC50 (nM)	
	HepG 2	Hep 3B
1	153.10±34.30**	180.6±31.63**
2	3161±207.55**	6250±358.93**
3	909.10±64.37**	1182±55.76**
4	1764±105.65**	2274±109.78**
5-Fluorouracil	5659±315.72	51709±370.67

All data were shown as means ±SD of three independent experiments. * $p < 0.05$, ** $p < 0.01$ compared with positive control.